4-Tert-butyl-2-chlorophenyl methyl dimethylamidophosphate

Inchi: InChI=1S/C13H21ClNO3P/c1-13(2,3)10-7-8-12(11(14)9-10)18-19(16,17-6)15(4)5/h7-9H,

InchiKey: DHKSNLDSXLVWFF-UHFFFAOYSA-N

Formula: C13H21ClNO3P

SMILES: COP(=O)(Oc1ccc(C(C)(C)C)cc1Cl)N(C)C

Mol. weight [g/mol]: 305.74

CAS: 14163-82-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.35		Crippen Method
logp	4.332		Crippen Method
mcvol	230.560	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14163827&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume